Direct transformations yielding the knight's move pattern in 3x3x3 arrays

Tendeiro, Jorge; ten Berge, Jos M. F.; Choulakian, V.

Published in:
Chemometrics and Intelligent Laboratory Systems

DOI:
10.1016/j.chemolab.2013.05.014

Chemometrics and Intelligent Laboratory Systems 129 (2013) 10–14

Contents lists available at ScienceDirect

Chemometrics and Intelligent Laboratory Systems

journal homepage: www.elsevier.com/locate/chemolab

Direct transformations yielding the knight's move pattern in $3 \times 3 \times 3$ arrays

Jorge N. Tendeiro [a,*], Jos M.F. Ten Berge [a], Vartan Choulakian [b]

[a] Heijmans Institute of Psychological Research, University of Groningen, Grote Kruisstraat 2/1, 9712 TS Groningen, The Netherlands
[b] Dépt. de Math./Statistique, Université de Moncton, Moncton NB E1A 3E9, Canada

ARTICLE INFO

Article history:
Received 23 November 2012
Received in revised form 8 April 2013
Accepted 26 May 2013
Available online 4 June 2013

Keywords:
Three-mode component analysis
Tucker transformations
Simplicity
Gröbner basis

ABSTRACT

Three-way arrays (or tensors) can be regarded as extensions of the traditional two-way data matrices that have a third dimension. Studying algebraic properties of arrays is relevant, for example, for the Tucker three-way PCA method, which generalizes principal component analysis to three-way data. One important algebraic property of arrays is concerned with the possibility of transformations to simplicity. An array is said to be transformed to a simple form when it can be manipulated by a sequence of invertible operations such that a vast majority of its entries become zero. This paper shows how $3 \times 3 \times 3$ arrays, whether symmetric or nonsymmetric, can be transformed to a simple form with 18 out of its 27 entries equal to zero. We call this simple form the "knight's move pattern" due to a loose resemblance to the moves of a knight in a game of chess. The pattern was examined by Kiers, Ten Berge, and Rocci. It will be shown how the knight's move pattern can be found by means of a numeric–algebraic procedure based on the Gröbner basis. This approach seems to work almost surely for randomly generated arrays, whether symmetric or nonsymmetric.

1. Introduction

Tucker [15] proposed an extension of component analysis to three-way arrays. Given an array $\underline{\mathbf{X}}$ of order $I \times J \times K$, Tucker's three-way PCA finds component matrices $\mathbf{A}$ $(I \times P)$, $\mathbf{B}$ $(J \times Q)$, $\mathbf{C}$ $(K \times R)$, and a $P \times Q \times R$ core array $\underline{\mathbf{G}}$ such that the function

$$\mathrm{h}\left(\mathbf{A}, \mathbf{B}, \mathbf{C}, \underline{\mathbf{G}}\right) = \left\|\mathbf{X} - \mathbf{A}\mathbf{G}\left(\mathbf{C}' \otimes \mathbf{B}'\right)\right\|^2 \tag{1}$$

is a minimum, where $\mathbf{X}$ is the $I \times JK$ matrix holding the K frontal slices of $\underline{\mathbf{X}}$, $\mathbf{G}$ is the $P \times QR$ matrix holding the R frontal slices of $\underline{\mathbf{G}}$, $'$ denotes the matrix transpose operator, and $\otimes$ is the Kronecker product.

As already noted by Tucker, the three-mode PCA model is not uniquely determined. Without loss of fit, the slices of the core can be premultiplied by $\mathbf{S}'$, postmultiplied by $\mathbf{T}$ and linearly combined by (elements from the columns of) $\mathbf{U}$, provided that $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ are postmultiplied by the inverse transformations $(\mathbf{S}')^{-1}$, $(\mathbf{T}')^{-1}$, and $(\mathbf{U}')^{-1}$, respectively. This means that transforming the matrix version $\mathbf{G}$ of the core into $\mathbf{S}'\mathbf{G}(\mathbf{U} \otimes \mathbf{T})$ is allowed, for any nonsingular $\mathbf{S}$, $\mathbf{T}$, and $\mathbf{U}$. Throughout this paper we will use the term "Tucker transformation" to refer to this type of mathematical operation.

Kiers et al. [6] pointed out that the non-uniqueness of the core can be suppressed by imposing constraints. Specifically, they examined the case $P = Q = R = 3$, when the core is constrained to be of the form

$$\mathbf{H} = \left[\begin{array}{ccc|ccc|ccc} x & 0 & 0 & 0 & 0 & d & 0 & f & 0 \\ 0 & 0 & b & 0 & y & 0 & e & 0 & 0 \\ 0 & a & 0 & c & 0 & 0 & 0 & 0 & z \end{array}\right], \tag{2}$$

holding at least 18 zero elements. Because there is a loose resemblance to the moves of a knight in a game of chess, this pattern is called the knight's move pattern (KMP). Kiers et al. [6] showed that any three nonsingular matrices $\mathbf{S}$, $\mathbf{T}$, and $\mathbf{U}$, transforming $\mathbf{G}$ to $\mathbf{S}'\mathbf{G}(\mathbf{U} \otimes \mathbf{T})$ while preserving the 18 zeros, are almost surely (rescaled) permutation matrices. This means that a Tucker three-way PCA with constrained core (2) has the property of essential uniqueness, just like Candecomp/Parafac [1,4].

The KMP (2) was first used by Rocci ([8], Eq. (13)). The same pattern was later rediscovered by a numerical procedure called Simplimax [5]. Originally, Simplimax allows rotating (i.e., Tucker-transforming) a core array to a simple pattern (i.e., a pattern with many zeros), when that is possible, after specifying the desired number of zeros (but not their positions). A modified version of Simplimax also allows fixing the desired target array. Monte Carlo studies using Simplimax indicate that random arrays of order $3 \times 3 \times 3$ admit a Tucker transformation

* Corresponding author. Tel.: +31 50 363 6953; fax: +31 50 363 6304.
E-mail addresses: j.n.tendeiro@rug.nl (J.N. Tendeiro), j.m.f.ten.berge@rug.nl (J.M.F. Ten Berge), vartan.choulakian@umoncton.ca (V. Choulakian).

0169-7439/$ – see front matter
http://dx.doi.org/10.1016/j.chemolab.2013.05.014

to the form (2) in most cases. This means that a model involving Eq. (2) as a core will often be a tautology, because the constraints need not be active.

The KMP also drew attention in other contexts. Firstly, it was treated by Wong [16] in the context of loglinear modeling. In addition, it was discussed by Rocci and Ten Berge [9] as an example of how the transformational freedom of the core can be used to attain a vast majority of zero elements. For many other examples, extreme forms of *simplicity* (many zero elements) that were first discerned with the help of Simplimax were given a solid footing by deriving closed-form solutions for the simplifying Tucker-transformation matrices, for example, Murakami et al. [7], Rocci and Ten Berge [9], Ten Berge and Kiers [10], and Tendeiro et al. [14]. For the KMP (Eq. (2)), however, nothing has been achieved so far. The present paper is aimed at filling this gap to some extent. For fully random (nonsymmetric) $3 \times 3 \times 3$ arrays, it will be shown how a Tucker transformation can be found which yields

$$\mathbf{H}_n = \left[\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 0 & 0 & d & 0 & f & 0 \\ 0 & 0 & a & 0 & 1 & 0 & e & 0 & 0 \\ 0 & b & 0 & c & 0 & 0 & 0 & 0 & 1 \end{array}\right]. \tag{3}$$

However, when the slices of the initial array $\underline{\mathbf{G}}$ are symmetric in at least one direction and random otherwise, it seems that we can attain the form

$$\mathbf{H}_s = \left[\begin{array}{ccc|ccc|ccc} h & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & h & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & h \end{array}\right]. \tag{4}$$

Each of these cases will be discussed in separate sections.

2. Fully random arrays

Suppose we have a $3 \times 3 \times 3$ array $\underline{\mathbf{G}}$, consisting of three slices $\mathbf{G}_i$, $i = 1, 2, 3$. We may premultiply all slices by the same nonsingular matrix $\mathbf{S}'$, postmultiply them by the same nonsingular matrix $\mathbf{T}$, and mix the slices by elements from the columns of a 3×3 nonsingular matrix $\mathbf{U}$, as will be specified in Eq. (5) below. Then a new array $\underline{\mathbf{H}}$ can be obtained, with slices

$$\mathbf{H}_i = \mathbf{S}'(u_{1i}\mathbf{G}_1 + u_{2i}\mathbf{G}_2 + u_{3i}\mathbf{G}_3)\mathbf{T}, \tag{5}$$

$i = 1, 2, 3$. The problem is how to attain a simplified form with slices

$$\mathbf{H}_1 = \begin{bmatrix} 0 & 0 & * \\ * & 0 & 0 \\ 0 & * & 0 \end{bmatrix}, \mathbf{H}_2 = \begin{bmatrix} 0 & * & 0 \\ 0 & 0 & * \\ * & 0 & 0 \end{bmatrix}, \tag{6}$$

with the * standing for free parameters, and $\mathbf{H}_3$ a diagonal matrix. This is not exactly the KMP but differs from it by permuting columns 2 and 3 of the slices and by switching slices 1 and 3, for reasons to be explained below. Upon defining the permutation matrix $\mathbf{P} = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$, with $\mathbf{P}^2 = \mathbf{P}' = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$, the question can equivalently be phrased as how to obtain, when that is possible, new slices $\mathbf{H}_1 = \mathbf{P}$, $\mathbf{H}_2 = \mathbf{P}^2\mathbf{D}$, and $\mathbf{H}_3 = \mathbf{E}$, with $\mathbf{D}$ and $\mathbf{E}$ diagonal matrices, to be chosen freely. Observe that the three nonzero entries of $\mathbf{H}_1$ can be constrained to unity by rescaling the lateral slices of $\underline{\mathbf{H}}$ (by multiplying the first, second, and third lateral slices of $\underline{\mathbf{H}}$ by $1/\mathbf{H}_1(2,1)$, $1/\mathbf{H}_1(3,2)$, and $1/\mathbf{H}_1(1,3)$, respectively). Define the slices we get when only the slabmix $\mathbf{U}$ is at work as

$$\mathbf{W}_i = u_{1i}\mathbf{G}_1 + u_{2i}\mathbf{G}_2 + u_{3i}\mathbf{G}_3, \tag{7}$$

$i = 1, 2, 3$. Define $\mathbf{A} = \mathbf{W}_1^{-1}\mathbf{W}_2$, $\mathbf{B} = \mathbf{W}_1^{-1}\mathbf{W}_3$, and $\mathbf{C} = \mathbf{W}_2^{-1}\mathbf{W}_3$.

Result 1. For a Tucker transformation to the KMP to exist it is necessary and sufficient that there is a real nonsingular matrix $\mathbf{U}$ such that

$$\mathrm{tr}(\mathbf{A}) = \mathrm{tr}\left(\mathbf{A}^{-1}\right) = \mathrm{tr}(\mathbf{B}) = \mathrm{tr}\left(\mathbf{B}^{-1}\right) = \mathrm{tr}(\mathbf{C}) = \mathrm{tr}\left(\mathbf{C}^{-1}\right) = 0. \tag{8}$$

Proof. Clearly, if the desired solution exists, we can permute and rescale it to have $\mathbf{S}'\mathbf{W}_1\mathbf{T} = \mathbf{P}$, $\mathbf{S}'\mathbf{W}_2\mathbf{T} = \mathbf{P}^2\mathbf{D}$, and $\mathbf{S}'\mathbf{W}_3\mathbf{T} = \mathbf{E}$. From $(\mathbf{S}'\mathbf{W}_1\mathbf{T})^{-1}\mathbf{S}'\mathbf{W}_2\mathbf{T} = \mathbf{P}'\mathbf{P}^2\mathbf{D} = \mathbf{PD}$ we see that

$$\mathbf{A} = \mathbf{TPDT}^{-1}. \tag{9}$$

From $(\mathbf{S}'\mathbf{W}_1\mathbf{T})^{-1}\mathbf{S}'\mathbf{W}_3\mathbf{T} = \mathbf{P}'\mathbf{E}$ we see that

$$\mathbf{B} = \mathbf{TP}'\mathbf{ET}^{-1}. \tag{10}$$

From $(\mathbf{S}'\mathbf{W}_2\mathbf{T})^{-1}\mathbf{S}'\mathbf{W}_3\mathbf{T} = \mathbf{D}^{-1}\mathbf{PE}$ we see that

$$\mathbf{C} = \mathbf{TD}^{-1}\mathbf{PET}^{-1}. \tag{11}$$

Above, two columns of the slices in the KMP were initially permuted. This was done to enable working with a permutation $\mathbf{P}$ that has diagonal zero. Because $\mathbf{P}$ has diagonal zero, so do $\mathbf{PD}$ in Eq. (9), $\mathbf{P}'\mathbf{E}$ in Eq. (10), and $\mathbf{D}^{-1}\mathbf{PE}$ in Eq. (11). It follows that $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, and their inverses have trace zero. Therefore, the six trace zero equations of (8) must be satisfied if the desired $\mathbf{S}$, $\mathbf{T}$, and $\mathbf{U}$ exist. This proves the necessity of the condition.

To prove sufficiency, suppose we can solve the six equations of Eq. (8), which are independent of $\mathbf{S}$ and $\mathbf{T}$, for a real $\mathbf{U}$. Then we obtain real matrices $\mathbf{W}_i$, $i = 1, 2, 3$, see Eq. (7), and real matrices $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$, see Eqs. (9), (10), and (11), respectively. Next, it can be verified that

$$\mathbf{ABCB} = \mathbf{TPDP}'\mathbf{ET}^{-1}\mathbf{TD}^{-1}\mathbf{PET}^{-1}\mathbf{TP}'\mathbf{ET}^{-1} = \mathbf{T}\left(\mathbf{PDP}'\mathbf{ED}^{-1}\mathbf{PEP}'\mathbf{E}\right)\mathbf{T}^{-1}$$

is an eigenequation because $\mathbf{PDP}'\mathbf{ED}^{-1}\mathbf{PEP}'\mathbf{E}$ is a diagonal matrix. Because $\mathbf{ABCB}$ is real, and its eigenvalues are real, we can find $\mathbf{T}$ (real) as a matrix of eigenvectors of $\mathbf{ABCB}$. Finally, we find $\mathbf{S}$ from $\mathbf{S}' = \mathbf{PT}^{-1}\mathbf{W}_1^{-1}$. Upon evaluating $\mathbf{S}'\mathbf{W}_i\mathbf{T}$, $i = 1, 2, 3$, final permutations and rescaling will yield the KMP. □

Details of the method of finding $\mathbf{U}$, $\mathbf{T}$, and $\mathbf{S}$ will be given in Appendix A (the program is written in Maple language). Unfortunately, a proof that the necessary and sufficient condition is satisfied almost surely has evaded us. However, numerical evidence to that effect is amply available, as will now be explained.

A Monte Carlo study with 1000 random arrays was performed. The entries of each array were uniformly drawn from the set of integers between −5 and 5; singular frontal slices were discarded and resampled until all three frontal slices were nonsingular. The procedure took around 34 min to complete using Maple 13 on a Linux machine with a 3.40 GHz processor and 8 Gb of RAM. Results revealed an essentially unique solution throughout. In fact, six solutions appear, which differ in permutations. So a unique solution seems to exist almost surely, in line with the uniqueness result of Kiers et al. [6]. The fact that all cases seem to admit a KMP, where Simplimax indicated success in most (but not all) cases, is new. Apparently, Simplimax sometimes needs more random starts than have been used in past studies. For instance, 2000 random starts are sometimes not enough. An additional advantage of the present approach is that its solution is exact. Simplimax minimizes a least squares function that attains values of zero in varying decimal places. The zeros we get from Maple are exact zeros.

3. Using the Gröbner basis to solve the system of linear equations

We start by observing that the system of six equations of Eq. (8) admits degenerate solutions which are of no practical use for the current problem (e.g., with rows of **U** identically equal to zero). A seventh equation (const $*$ Det(**U**) $-1 = 0$) was therefore added to prevent solutions with **U** singular. We set $u_{11} = u_{12} = u_{13} = 1$ for identification purposes, without loss of generality.

A general recipe for solving the system of seven equations in closed form has evaded us. Instead, we used a numerical procedure to estimate a solution based on the Gröbner basis with lexicographic order, see for instance Choulakian [2] and Cox et al. ([3], Ch. 2). The Gröbner basis of a set of polynomials is typically another set of polynomials which: (1) share the same roots with the original polynomials, and (2) are much easier to solve for with respect to the unknowns using an elimination procedure. In the context of our problem, while finding the zeros of the original polynomials was revealed as unfeasible, it turned out to be very easy to find u_{21}, ..., u_{33} as zeros of the polynomials in the Gröbner basis of {trace(**A**), trace($\mathbf{A}^{-1}$), trace(**B**), trace($\mathbf{B}^{-1}$), trace(**C**), trace($\mathbf{C}^{-1}$), const $*$ Det(**U**) -1}.

4. When slices are symmetric

When slices of $\underline{\mathbf{G}}$ are symmetric in one direction, an initial Tucker transformation exists that renders the array fully symmetric, of the form

$$\mathbf{G}_s = \left[\begin{array}{ccc|ccc|ccc} 1+x & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1+y & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1+z \end{array}\right] \tag{12}$$

(see Ten Berge and Sidiropoulos ([11], p. 406) or Tendeiro ([13], p. 76)). Because this array is fully symmetric, and so is the targeted pattern $\mathbf{H}_s$ of (4), Tendeiro conjectured that a Tucker transformation of $\mathbf{G}_s$ to $\mathbf{H}_s$ might involve $\mathbf{S} = \mathbf{T} = \mathbf{U}$. This will now be proven.

Result 2. When a fully symmetric array like Eq. (12) can be transformed to a KMP that is also fully symmetric, we have $\mathbf{S} = \mathbf{T} = \mathbf{U}$, except for sign changes, almost surely.

Proof. Let the columns of **U** define linear combinations $\mathbf{G}_1^*$, $\mathbf{G}_2^*$, and $\mathbf{G}_3^*$ of the three frontal slices of $\mathbf{G}_s$. Let $\mathbf{H}_i = \mathbf{S}'\mathbf{G}_i^*\mathbf{T}$, $i = 1,2,3$, be the frontal slices of the fully symmetric array **H** that has the KMP. Then the symmetry of $\mathbf{H}_i$ implies symmetry of $(\mathbf{T}')^{-1}\mathbf{S}'\mathbf{G}_i^*$, $i = 1,2,3$. Define $\mathbf{N} = (\mathbf{T}')^{-1}\mathbf{S}'$. The symmetry of $\mathbf{NG}_1^*$, $\mathbf{NG}_2^*$, and $\mathbf{NG}_3^*$ implies nine equations, that can be translated into orthogonality of the vector **n**, holding the rows of **N** stacked below each other, to the columns of a 9 × 9 matrix that is constructed according to the method of Ten Berge and Stegeman ([12], Eq. (4)). In our case, using Eq. (12), that matrix is

$$\begin{bmatrix} -1 & -1 & 0 & -1 & -1 & 0 & -1 & -1 & 0 \\ -1 & -1 & 0 & -1-y & -1 & 0 & -1 & -1 & 0 \\ -1 & -1 & 0 & -1 & -1 & 0 & -1 & -1-z & 0 \\ 1+x & 0 & -1 & 1 & 0 & -1 & 1 & 0 & -1 \\ 1 & 0 & -1 & 1 & 0 & -1 & 1 & 0 & -1 \\ 1 & 0 & -1 & 1 & 0 & -1 & 1 & 0 & -1-z \\ 0 & 1+x & 1 & 0 & 1 & 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 1 & 1+y & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 1 \end{bmatrix}.$$

Almost surely, the only vector orthogonal to the columns of this matrix is the vector holding the columns of $\mathbf{I}_3$ or $-\mathbf{I}_3$. It follows that $\mathbf{S} = \mathbf{T}$ or $\mathbf{S} = -\mathbf{T}$. The same method can be used to prove that $\mathbf{S} = \mathbf{U}$ up to sign. □

Inspection of 1000 cases where the procedure was applied to arrays with symmetric slices revealed that this is indeed what happens. In fact, a different procedure based on equality of **S**, **T**, and **U** was also derived and proved equally successful. Details are available upon request but will not be given here because the general procedure for fully random arrays, discussed in Appendix A, also handles the cases of symmetric arrays.

The Tucker transformation for symmetric arrays does not immediately return a KMP of the form (4). Instead, simulations showed that the pattern

$$\left[\begin{array}{ccc|ccc|ccc} h_1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & h_2 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & h_3 \end{array}\right] \tag{13}$$

with h_1, h_2, and h_3 different, arises consistently. Transforming form (13) to the KMP requires some postprocessing. Let

$$\mathbf{D}_h = \begin{bmatrix} h_1^{-1/3} & 0 & 0 \\ 0 & h_2^{-1/3} & 0 \\ 0 & 0 & h_3^{-1/3} \end{bmatrix}. \tag{14}$$

Pre and postmultiplying the slices of Eq. (13) by $\mathbf{D}_h$, and mixing (here rescaling) them by columns of $\mathbf{D}_h$ produces new slices

$$\mathbf{H}_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & h^{-1/3} \\ 0 & h^{-1/3} & 0 \end{bmatrix}, \mathbf{H}_2 = \begin{bmatrix} 0 & 0 & h^{-1/3} \\ 0 & 1 & 0 \\ h^{-1/3} & 0 & 0 \end{bmatrix}, \tag{15}$$
$$\mathbf{H}_3 = \begin{bmatrix} 0 & h^{-1/3} & 0 \\ h^{-1/3} & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

where $h = h_1h_2h_3$. Multiplying these slices by $h^{1/3}$ yields an array like Eq. (13) but with parameters h_1, h_2, and h_3 rescaled to $h^{1/3}$, which yields a solution of the form (4). This shows that we may set h_1, h_2, and h_3 equal to their geometric mean without loss of generality. The bottom line is that, almost surely, a (partially) symmetric 3 × 3 × 3 array seems to admit a Tucker transformation to an array that has 18 zeros and that depends on a single parameter. This can be viewed as a "canonical form" for such arrays. It is not known if this form generalizes to higher order symmetric arrays.

5. An example

We illustrate the general procedure with an example (the results can be reproduced using the code shown in Appendix A). Consider array **G**,

$$\left[\begin{array}{ccc|ccc|ccc} 1 & 0 & -2 & 3 & -5 & -2 & -3 & 2 & 0 \\ 0 & 2 & 3 & 1 & 4 & -2 & -1 & 0 & 2 \\ -1 & 1 & 1 & 0 & 2 & 3 & 3 & 1 & 2 \end{array}\right] \tag{16}$$

with frontal slices $\mathbf{G}_1$, $\mathbf{G}_2$, and $\mathbf{G}_3$. We can compute $\mathbf{W}_i = \mathbf{G}_1 + u_{2i}\mathbf{G}_2 + u_{3i}\mathbf{G}_3$ $(i = 1, 2, 3)$, $\mathbf{A} = \mathbf{W}_1^{-1}\mathbf{W}_2$, $\mathbf{B} = \mathbf{W}_1^{-1}\mathbf{W}_3$, and $\mathbf{C} = \mathbf{W}_2^{-1}\mathbf{W}_3$; observe that these matrices are functions of u_{21}, u_{22}, u_{23}, u_{31}, u_{32}, and u_{33}. It is now possible to construct the seven polynomials of which the six u variables (plus the variable that suppresses singularity of **U**) are the desired solutions. The roots of the polynomials from the associated Gröbner basis are:

$$\begin{array}{lll} u_{21} = -.6758206016 & u_{22} = .5539638606 & u_{23} = .08965478826 \\ u_{31} = -.3839477779 & u_{32} = .9137741095 & u_{33} = -.9539026181. \end{array} \tag{17}$$

With $\mathbf{U}$ determined, it is straightforward to find $\mathbf{T}$ as the eigenvector matrix of $\mathbf{ABCB}$ and $\mathbf{S} = (\mathbf{PT}^{-1}\mathbf{W}_1^{-1})'$:

$$\mathbf{S} = \begin{bmatrix} .3276 & -.2674 & -.1890 \\ .2164 & -.3310 & .1245 \\ -.1014 & -.4362 & -.2135 \end{bmatrix}, \tag{18}$$

$$\mathbf{T} = \begin{bmatrix} .9325 & .0626 & .2074 \\ .0984 & -.6986 & .9230 \\ -.3475 & .7127 & .3240 \end{bmatrix}. \tag{19}$$

The simplified array $[\mathbf{H}_1|\mathbf{H}_2|\mathbf{H}_3] = \mathbf{S}'[\mathbf{G}_1|\mathbf{G}_2|\mathbf{G}_3]$ $(\mathbf{U}\otimes\mathbf{T})$ is now readily available, that is,

$$\begin{aligned} \mathbf{H}_1 &= \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \\ \mathbf{H}_2 &= \begin{bmatrix} 0 & -.7016 & 0 \\ 0 & 0 & -3.1649 \\ -.4008 & 0 & 0 \end{bmatrix}, \\ \mathbf{H}_3 &= \begin{bmatrix} 1.9665 & 0 & 0 \\ 0 & .5873 & 0 \\ 0 & 0 & .8883 \end{bmatrix}. \end{aligned} \tag{20}$$

Final permutation and rescaling transformations to simple form (3) are now easy to perform.

6. Simplifying 6 × 3 × 3 arrays

Rocci and Ten Berge [9] have shown that Tucker transformations to simplicity for a $P \times Q \times R$ array may also be used to simplify a $P \times Q \times (PQ - R)$ array. They gave an example of how to simplify a $3 \times 3 \times 7$ array by using the results that simplified the “complementary” $3 \times 3 \times 2$ array. Likewise, having obtained a solution to simplify $3 \times 3 \times 3$ arrays (nonsymmetric), we can now simplify $3 \times 3 \times 6$ arrays. Specifically, start by rewriting a given $3 \times 3 \times 6$ array $\underline{\mathbf{G}}$ into a 9×6 matrix $\mathbf{G}^*$ by vectorizing rowwise each 3×3 slice of $\underline{\mathbf{G}}$. Next, compute the 9×3 orthogonal complement of $\mathbf{G}^*$, say $\mathbf{G}^*{}_c$, which is a vectorized form of a $3 \times 3 \times 3$ array. Using the main result in this paper we can now simplify this $3 \times 3 \times 3$ array into the rowwise vectorized simple form

$$\mathbf{H}_c^* = \left(\mathbf{S}'\otimes\mathbf{T}'\right)\mathbf{G}_c^*\mathbf{U} = \left[\begin{array}{ccc} 0 & 0 & d \\ 0 & a & 0 \\ 1 & 0 & 0 \\ \hline 1 & 0 & 0 \\ 0 & 0 & e \\ 0 & b & 0 \\ \hline 0 & c & 0 \\ 1 & 0 & 0 \\ 0 & 0 & f \end{array}\right]. \tag{21}$$

As a final step, compute $\mathbf{H}^*$, the 9×6 orthogonal complement of $\mathbf{H}^*{}_c$:

$$\mathbf{H}^* = \begin{bmatrix} 0 & -e/d & 0 & 0 & 0 & -f/d \\ 0 & 0 & -b/a & -c/a & 0 & 0 \\ -1 & 0 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \tag{22}$$

where $\mathbf{H}^*$ is the vectorized version of the $3 \times 3 \times 6$ array $\underline{\mathbf{H}}$, which is the simple form of $\underline{\mathbf{G}}$.

Now, observe that $(\mathbf{G}^*{}_c)'\mathbf{G}^* = \mathbf{0}$ implies

$$\mathbf{U}'\left(\mathbf{G}_c^*\right)'(\mathbf{S}\otimes\mathbf{T})(\mathbf{S}\otimes\mathbf{T})^{-1}\mathbf{G}^* = \left(\mathbf{H}_c^*\right)'(\mathbf{S}\otimes\mathbf{T})^{-1}\mathbf{G}^* = \mathbf{0}$$

so the columns of $\mathbf{H}^*{}_c$ are orthogonal to the columns of $(\mathbf{S}\otimes\mathbf{T})^{-1}\mathbf{G}^*$, and therefore the columns of $\mathbf{H}^*$ are in the column space of $(\mathbf{S}\otimes\mathbf{T})^{-1}\mathbf{G}^*$. Hence, there exists an $\mathbf{M}$ (6×6) such that $(\mathbf{S}\otimes\mathbf{T})^{-1}\mathbf{G}^*\mathbf{M}$ has zeros in the same places as $\mathbf{H}^*$. It is easy to find $\mathbf{M}$ as the inverse of the lower 6×6 submatrix of $(\mathbf{S}\otimes\mathbf{T})^{-1}\mathbf{G}^*$. This shows how to transform a $6 \times 3 \times 3$ array to simplicity, having only 12 nonzero elements.

A practical illustration of the procedure just described might be helpful. Consider the $3 \times 3 \times 6$ array $\underline{\mathbf{G}}$ whose 9×6 rowwise vectorized $\mathbf{G}^*$ form is

$$\mathbf{G}^* = \begin{bmatrix} -2.2 & -40.4 & 10.2 & -37.4 & 3.8 & 8.8 \\ -13.2 & -7.8 & 16.4 & -15.4 & -4.2 & -4.4 \\ 5.5 & -30.1 & -10.3 & -34.1 & -25.6 & 15.4 \\ -17.6 & -11.0 & -8.8 & -11.0 & 8.8 & -2.2 \\ -8.8 & 11.0 & 4.4 & 13.2 & -15.4 & 0.0 \\ 6.6 & -15.4 & -11.0 & -8.8 & 0.0 & 8.8 \\ -8.8 & -19.8 & 2.2 & -6.6 & 17.6 & 4.4 \\ -11.0 & -4.4 & -13.2 & -19.8 & 11.0 & -2.2 \\ 13.2 & -11.0 & 8.8 & -17.6 & -17.6 & 2.2 \end{bmatrix}. \tag{23}$$

It is easy to verify that the orthogonal complement of $\mathbf{G}^*$, $\underline{\mathbf{G}}_c$, is given by Eq. (16). Hence, a simple form for $\underline{\mathbf{G}}$ can be computed as $(\mathbf{S}\otimes\mathbf{T})^{-1}\mathbf{G}^*\mathbf{M}$, where $\mathbf{S}$ and $\mathbf{T}$ are respectively given by Eqs. (18) and (19), and $\mathbf{M}$ is the inverse of the lower 6×6 submatrix of $(\mathbf{S}\otimes\mathbf{T})^{-1}\mathbf{G}^*$. The final result is

$$\begin{bmatrix} 0 & -.2986 & 0 & 0 & 0 & -.4517 \\ 0 & 0 & -4.5108 & -.5713 & 0 & 0 \\ -1 & 0 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \tag{24}$$

which is a simple form with only 12 nonzero elements.

7. Discussion

Solving the equations that imply the KMP for (partially) symmetric $3 \times 3 \times 3$ arrays seems possible almost surely. What is missing is a proof that our six equations admit a real solution almost surely. We have merely observed that it never seems to fail for random data, with or without constraints of symmetry.

The simplicity results for $3 \times 3 \times 3$ arrays (18 zeros) and for $3 \times 3 \times 6$ arrays (42 zeros) do give a vast majority of zeros. However, it is not known whether these results are maximum simplicity results. Conceivably, these arrays admit Tucker transformations that yield even more zeros.

Appendix A. Maple code for solving the system of seven equations

The first part of the code shows how to find the Gröbner basis for the set of seven polynomials of interest, for a given array.

```
restart:
with(LinearAlgebra): with(Groebner): with(stats): with(ArrayTools):
Digits:=100:

# Enter 3x3x3 array:
G1 := Matrix(3,3,[1,0,-2,0,2,3,-1,1,1]):
G2 := Matrix(3,3,[3,-5,-2,1,4,-2,0,2,3]):
G3 := Matrix(3,3,[-3,2,0,-1,0,2,3,1,2]):

U := Matrix([[1,1,1],[u21,u22,u23],[u31,u32,u33]]):
W1 := G1 + u21*G2 + u31*G3:
W2 := G1 + u22*G2 + u32*G3:
W3 := G1 + u23*G2 + u33*G3:
# The adjoint is used instead of the inverse to simplify computations:
A := simplify(Adjoint(W1).W2):
B := simplify(Adjoint(W1).W3):
C := simplify(Adjoint(W2).W3):

# The 7 polynomials:
pol1 := Trace(A):
pol2 := Trace(Adjoint(A)):
pol3 := Trace(B):
pol4 := Trace(Adjoint(B)):
pol5 := Trace(C):
pol6 := Trace(Adjoint(C)):
pol7 := const * Determinant(U)-1:

# Get the Groebner basis:
poly  := [pol1,pol2,pol3,pol4,pol5,pol6,pol7]:
polyG := Basis(poly, plex(u21,u22,u23,u31,u32,u33,const)):
```

Next, variables u_{21} through u_{33} can be extracted from the Gröbner basis by an elimination procedure:

```
constSol := fsolve(polyG[1])[1]:
u33Sol := fsolve(subs(const = constSol, polyG[2]))[1]:
u32Sol := fsolve(subs(const = constSol, u33 = u33Sol, polyG[3])):
u31Sol := fsolve(subs(const = constSol, u33 = u33Sol, u32=u32Sol,
polyG[4])):
u23Sol := fsolve(subs(const = constSol, u33 = u33Sol, u32=u32Sol,
u31=u31Sol, polyG[5])):
u22Sol := fsolve(subs(const = constSol, u33 = u33Sol, u32=u32Sol,
u31=u31Sol, u23=u23Sol, polyG[6])):
u21Sol := fsolve(subs(const = constSol, u33 = u33Sol, u32=u32Sol,
u31=u31Sol, u23=u23Sol, u22=u22Sol, polyG[7])):
```

At this point **U** is available. Finding matrices **S** and **T** can be done as follows:

```
W1Sol := G1 + u21Sol *G2 + u31Sol *G3:
W2Sol := G1 + u22Sol *G2 + u32Sol *G3:
W3Sol := G1 + u23Sol *G2 + u33Sol *G3:
ASol := MatrixInverse(W1Sol).W2Sol:
BSol := MatrixInverse(W1Sol).W3Sol:
CSol := MatrixInverse(W2Sol).W3Sol:
T := Re(Eigenvectors(ASol.BSol.CSol.BSol)[2]):
P := Matrix([[0,0,1],[1,0,0],[0,1,0]]):
S := Transpose(P.MatrixInverse(T).MatrixInverse(W1Sol)):
```

The slices of the rotated array in simple form are given by the commands:

```
H1 := Transpose(S).W1Sol.T:
H2 := Transpose(S).W2Sol.T:
H3 := Transpose(S).W3Sol.T:
```

Finally, it remains to perform rescaling and permutations to identify matrices H1, H2, and H3 with the simple form of Eq. (3).

References

[1] J.D. Carroll, J.J. Chang, Analysis of individual differences in multidimensional scaling via an n-way generalization of Eckart–Young decomposition, Psychometrika 35 (1970) 283–319.
[2] V. Choulakian, Some numerical results on the rank of generic three-way arrays over R, SIAM Journal on Matrix Analysis and Applications 31 (2010) 1541–1551.
[3] D. Cox, J. Little, D. O'Shea, Ideals, Varieties, and Algorithms, 3rd ed. Springer, New York, 2007.
[4] R.A. Harshman, Foundations of the Parafac procedure: models and conditions for “explanatory” multimode factor analysis, UCLA Working Papers in Phonetics, 16, 1970, pp. 1–84.
[5] H.A.L. Kiers, Three-way Simplimax for oblique rotation of the three-mode factor analysis core to simple structure, Computational Statistics and Data Analysis 28 (1998) 307–324.
[6] H.A.L. Kiers, J.M.F. Ten Berge, R. Rocci, Uniqueness of three-mode factor models with sparse cores: the 3 × 3 × 3 case, Psychometrika 62 (1997) 349–374.
[7] T. Murakami, J.M.F. Ten Berge, H.A.L. Kiers, A case of extreme simplicity of the core matrix in three-mode principal component analysis, Psychometrika 63 (1998) 255–261.
[8] R. Rocci, Three-mode factor analysis with binary code and orthonormality constraints, Journal of the Italian Statistical Society 3 (1992) 413–422.
[9] R. Rocci, J.M.F. Ten Berge, Transforming three-way arrays to maximal simplicity, Psychometrika 67 (2002) 351–365.
[10] J.M.F. Ten Berge, H.A.L. Kiers, Simplicity of core arrays in three-way principal component analysis and the typical rank of $P \times Q \times 2$ arrays, Linear Algebra and Its Applications 294 (1999) 169–179.
[11] J.M.F. Ten Berge, N.D. Sidiropoulos, On uniqueness in Candecomp/Parafac, Psychometrika 67 (2002) 399–409.
[12] J.M.F. Ten Berge, A. Stegeman, Symmetry transformations for square sliced three-way arrays, with applications to their typical rank, Linear Algebra and its Applications 418 (2006) 215–224.
[13] J.N. Tendeiro, Some Mathematical Results on Three-way Component Analysis (PhD thesis) University of Groningen, The Netherlands, 2010.
[14] J.N. Tendeiro, J.M.F. Ten Berge, H.A.L. Kiers, Simplicity transformations for three-way arrays with symmetric slices, and applications to Tucker-3 models with sparse core arrays, Linear Algebra and its Applications 430 (2009) 924–940.
[15] L.R. Tucker, Some mathematical notes on three-mode factor analysis, Psychometrika 31 (1966) 279–311.
[16] R.S.-K. Wong, Multidimensional association models. A multilinear approach, Sociological Methods & Research 30 (2001) 197–240.